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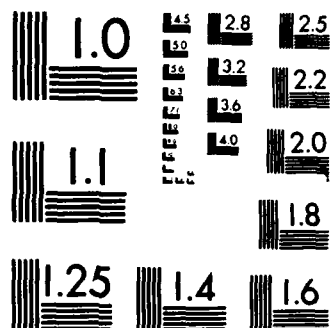
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A Study of Chaos and Mixing in Rayleigh-Taylor and Richtmyer-Meshkov Unstable Interfaces

C. L. Gardner, J. Glimm, J. Grove, O. McBryan
R. Menikoff, D. H. Sharp and Q. Zhang

Research and Development Report

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A STUDY OF CHAOS AND MIXING IN RAYLEIGH-TAYLOR AND RICHTMYER-MESHKOV UNSTABLE INTERFACES

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ABSTRACT

A program for the study of chaotic mixing layers produced by unstable interfaces is proposed and recent progress of the authors within this program is presented.

1. Introduction

The authors
Instabilities of fluid interfaces give rise to entrainment and to a chaotic mixing layer. This report has three purposes. We discuss the general features of such chaotic mixing layers, we formulate a scientific program for their study and we report on *their* recent progress of the authors in carrying out portions of this program.

The Rayleigh-Taylor instability is driven by an inertial or gravitational force accelerating an interface between fluids of differing densities. Thus with the heavy fluid above the lighter fluid a flat

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→ (horizontal) interface in a gravitational field is in a position of unstable equilibrium. Small disturbances grow, producing bubbles of light fluid rising in the heavy fluid and spikes or droplets of heavy fluid falling in the light fluid. The Richtmyer-Meshkov instability is produced by a shock wave hitting an interface (a contact discontinuity or material boundary) separating fluids of differing densities. Assuming a planar shock wave normally incident on an interface slightly perturbed from planar, the initial disturbances in the interface are again unstable, and grow with time. < —

There are many other examples of related interfacial instabilities. In certain parameter ranges, the displacement of oil by water in an oil reservoir is unstable and fingers of water penetrate into the oil. This is known as the Taylor-Saffman instability. The Kelvin-Helmholtz instability refers to the roll up of a vortex sheet or slip surface. Phase transitions in a supersaturated or metastable medium lead to dendritic growth of finger-like instabilities. Interfacial mixing processes are important, interesting, and difficult to study. They possess a number of common features which unify them as a single aspect of the broader study of chaos.

It is well known that turbulence in two dimensions is dominated by the growth and transfer of energy to large scale structures. This dominance of large scale motion is a common feature of all interface mixing processes, and results from nonlinear mode competition, as we shall see. It is convenient to identify the most important time regimes which characterize interface mixing and chaos.

A small amplitude disturbance can be characterized as a perturbation of a planar interface. After a linearization (in powers of the amplitude), the equations can be solved, and for certain parameter values show exponential growth. The regions in parameter space of exponential growth (the unstable regions) have been studied in detail (Chandrasekar³) and depend on the specific equations in question. As the instabilities grow, they give rise to characteristic modes. These modes are in the form of fingers or spikes for all problems mentioned above, except for the Kelvin-Helmholtz instability, in which case the elementary modes are vortices. After a further period of time, these modes no longer grow independently, but interact, compete and merge, thereby leading to the growth of large scale structures from small ones. Finally a chaotic regime emerges, in which the individual modes are difficult to identify.

2. A Scientific Program

As with any complex problem, the chaotic entrainment produced by an unstable interface is best studied by the use of several different approaches and in each approach by dividing the problem into subproblems. The first goal of a mixing layer theory is to predict its thickness as a function of time. If it is possible to specify the reference frame of the original unperturbed interface, then it is also of interest to determine the growth of each edge of the mixing layer separately, relative to this reference frame. Within the mixing layer, a theory should predict the relative mass fraction of the two fluids. Also the surface area or the fractal dimension of the convoluted interface is of interest. Further questions arise in specific contexts.

A direct application of the fluid equations to the chaotic regime is untractable and a simplified statistical description of the problem is essential. The main feature which the statistical model must

predict is the transfer of disturbances from small to large scales. The main steps in the scientific program are as follows:

- (a) Formulation of the statistical model. The model should be simple enough to be effectively solvable (step (c)), and complex enough to agree with the statistical behavior of the original equations (step (d) and (e)).
- (b) Setting the parameters of the statistical model as a function of the parameters of the fluid model. Any parameters not set in this manner from first principles are then adjustable parameters to be set during the validation steps (d) and (e) below. In view of expected difficulties in the computations and experiments, it is desirable to have as few adjustable parameters as possible, for example none.
- (c) An analytic or numerical study of the statistical model. It is necessary to determine qualitative or quantitative properties of the model which can be tested in steps (d) and (e). If the tests succeed, then further properties of the model can be expected to represent properties of the original problem as well.
- (d) Direct numerical simulation of the full fluid equations to confirm predictions which may emerge from (c). If the simulations were possible in situations of primary interest (fully developed chaos) there would be no great need to develop the model. Usually this is not the case, and the numerical simulations may test the model in a simpler situation, such as with only a moderate number of interacting modes, and only in two dimensions.
- (e) Laboratory experiments to establish the validity of the model and of the predicted behavior of its solutions. Again if necessary, this step can be simplified by carrying out the test in some relatively accessible range of experimental parameters.

For two dimensional turbulence, the Kolmogoroff spectral analysis provides a statistical model, which does predict the transfer of energy from small to large scales. For the Taylor-Saffman instability, a phenomenological velocity dependent diffusion tensor is used to model mixing layer growth. We present below the Sharp-Wheeler^{13,14} model to represent Rayleigh-Taylor mixing layer growth. Because of the similarities of this to the Richtmyer-Meshkov mixing layer, it would be of interest to modify this model to be applicable to the Richtmyer-Meshkov instability.

The Sharp-Wheeler model is a simplified description of the bubble interface, which is the boundary of the mixing layer adjacent to the ambient heavy fluid. The interface is required to be piecewise constant and single valued in this model. In two dimensions, the interface is represented by a function $z = z(x, t)$. At a fixed time t , each constant x interval represents a bubble. There are two parameters which determine the dynamics of the bubbles. A single bubble with height $z = z(t)$ moves according to the law

$$\dot{z}(t) = c_1 (gr(t))^{\frac{1}{2}}$$

where $r(t)$ is the bubble radius, g is the gravitational constant and c_1 is a dimensionless parameter. The determination of c_1 depends only on a single noninteracting mode of the full fluid equations, which we

refer to as the one body problem.

When the larger of two adjacent bubbles moves sufficiently far ahead of its smaller neighbor, the two bubbles are merged. This means that two adjacent intervals with distinct constant heights z are combined into a single interval, with the new height set to conserve area (mass). The merger criterion is

$$c_2 r_1(t) \leq z_2(t) - z_1(t)$$

provided

$$r_1(t) \leq r_2(t),$$

where c_2 is another dimensionless parameter.

3. Results for the Richtmyer-Meshkov Instability

Results from Grove¹⁰ apply to step (d) above: the direct numerical solution of the two fluid Euler compressible equations for multi-mode initial data. The front tracking algorithm⁴ allows enhanced numerical resolution per grid cell, in contrast to earlier computations of Youngs.¹⁵

The Richtmyer-Meshkov instability occurs when an interface between two different gases is accelerated by a collision with an incident shock wave. The direct simulation of this instability as for the Rayleigh-Taylor instability is based on a numerical solution to the Euler equations for a non-viscous, non-heat conducting gas.

(Conservation of mass)

$$\rho_t + (\rho u)_x + (\rho v)_y = 0, \quad (1a)$$

(Conservation of momentum)

$$(\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y = \rho g_1, \quad (1b)$$

$$(\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y = \rho g_2, \quad (1c)$$

(Conservation of energy)

$$\left\{ \rho \left[\frac{1}{2} q^2 + e \right] \right\}_t + \left\{ \rho u \left[\frac{1}{2} q^2 + i \right] \right\}_x + \left\{ \rho v \left[\frac{1}{2} q^2 + i \right] \right\}_y = \rho u g_1 + \rho v g_2. \quad (1d)$$

The variables u and v are the x and y components of the gas velocity at the point (x, y) , $q^2 = u^2 + v^2$, and g_1 and g_2 are the x and y coordinates of the gravitational acceleration vector \mathbf{g} . The thermodynamic variables ρ , e , p and $i = e + \frac{p}{\rho}$ are respectively the density, specific internal energy, pressure and specific enthalpy of the gas. The thermodynamic variables for each gas are related by a caloric equation of state

$$e = f(\rho, p). \quad (2)$$

In general this equation of state will be different for the two gases on opposite sides of the gas interface. The numerical examples described below use a polytropic equation of state,

$$e = \frac{p}{(\gamma - 1)\rho}, \quad (2')$$

where the ratio between the specific heats γ is a constant satisfying $1 < \gamma \leq \frac{5}{3}$.

Since the Richtmyer-Meshkov instability is concerned with the unstable modes excited by the shock wave collision, the simulation is taken to be on a horizontal cross section, and the effects of gravity are neglected, thus $g_1 = g_2 = 0$.

The front tracking algorithm solves the system of equations (1) by using a finite difference method coupled to a shock fitting algorithm. The solution near the tracked waves is found by solving Riemann problems across the surfaces of discontinuity in order to find the position and the states near the wave at time $t + \Delta t$. This information is then used as boundary data for a finite difference method for the solution away from the tracked interface. See^{8,7,4,9} for more details of the method.

The Richtmyer-Meshkov instability simulation is initialized at a time shortly before the incident shock wave reaches the gas interface. The incident shock is taken to be planar, and the contact discontinuity interface is given an initial geometry specified by input. If a single mode is to be isolated this initial geometry is that of a sine wave of a single period across the computational domain. The gas interface is assumed to be at rest with respect to the gas ahead of the incident shock so that prior to the collision between the shock wave and the gas interface the solution is piecewise constant. This piecewise constancy is lost as the shock interacts with the curved contact discontinuity interface.

Since the two interacting waves are tracked, it is necessary to resolve the diffracted wave patterns that are produced at the point of collision between the two waves. In the simulation used here, these diffraction patterns are resolved using shock polars. Briefly, the interacting waves are approximated by their tangents near the point of collision between the incident shock wave and the gas interface, and the nearby states are approximated by states that are constant between the interacting waves. It is then assumed that there is a frame of reference in which this local approximation is a steady flow. The analysis of the interaction between a planar shock wave and a planar contact discontinuity is well known.^{1,2,9} The type of diffraction pattern that is observed is a function of the strengths of the interacting waves, the angle at which the two waves meet, and the equations of state for the two gases. The simplest of these diffraction patterns consists of the incident shock wave and contact discontinuity, a single reflected wave that is either a shock or a centered rarefaction wave, a transmitted shock wave, and a deflected gas interface behind the point of interaction. This so called regular shock diffraction is observed provided the angle between the interacting waves is sufficiently small, this case occurs if the amplitude of the initial contact discontinuity is not too large.

In the local approximation, there are two generic streamlines associated with the regular diffraction pattern. One corresponds to the flow of gas particles through the incident shock and then through the reflected wave, and the other to the flow through the transmitted shock. These streamlines correspond to the gas flow on opposite sides of the contact discontinuity interface. The condition that the flow is piecewise constant and steady requires that these two stream lines are parallel ahead and behind the point of diffraction. Thus the net turn of the flow through the incident shock and reflected

wave must equal the turn of the flow through the transmitted shock. If the states ahead of the incident shock on both sides of the gas interface are known, and the strength of the incident shock (as say measured by the pressure jump across the shock) is also given, then the Rankine-Hugoniot relations provide a set of algebraic equations that contain as a solution the states of the gases behind the incident waves together with the angles between the interacting waves. This calculation of piecewise constant steady flows of this and similar types based on the turning of the flow through various waves is commonly called shock polar analysis. The details are too lengthy to repeat here, and the interested reader is referred to⁵ and the above cited references for more details. Figure 1, shows a representative shock diffraction pattern along with a pair of generic streamlines for the case of a reflected shock.

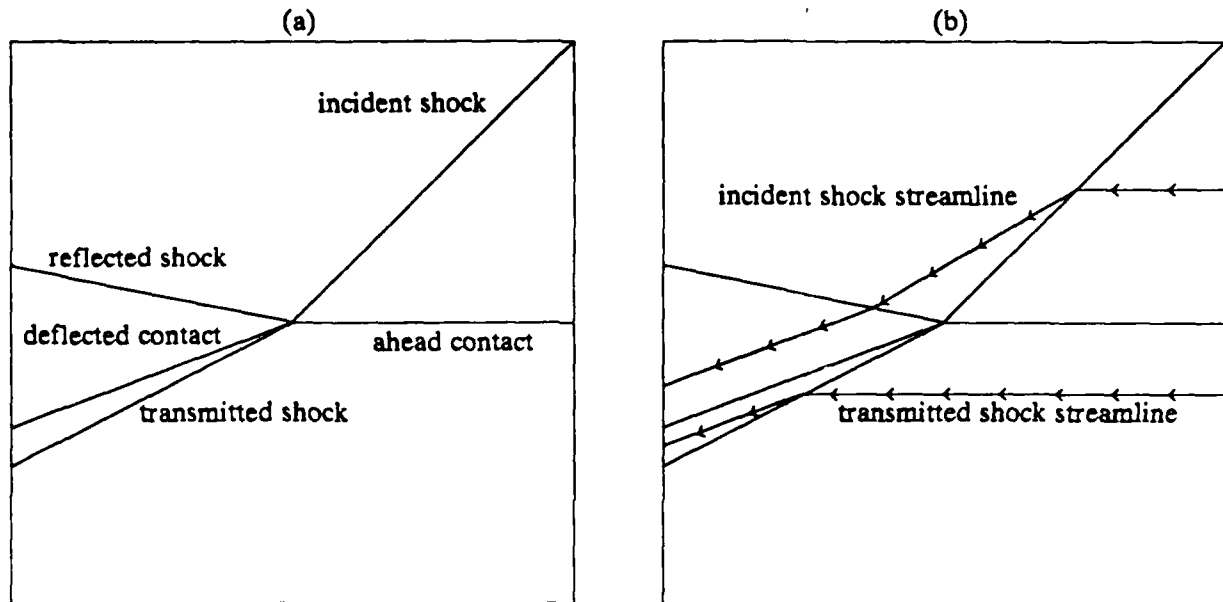


Fig. 1. A shock wave-contact discontinuity collision that produces a single reflected shock. The reaction occurs in air modeled as a polytropic gas with $\gamma = 1.402$. The gas on the transmitted shock side of the ahead contact discontinuity is four times as dense as the gas on the incident shock side. The angle between the incident shock and the ahead contact discontinuity is 45° , and the ratio of the pressures across the incident shock is 10. The flow is turned by about 30.3° through the incident shock, -9.8° through the reflected shock, and 20.5° through the transmitted shock.

The application of this shock polar analysis to the direct simulation of the shock contact collision consists of calculating at each time step a new piecewise constant steady diffraction pattern based on the changing angles between the incident waves. The transformation from the locally steady configuration to the global reference frame for the entire simulation is found by calculating an intersection between the two propagated sections of the incident shock wave and contact discontinuity. This intersection defines the position of the point of shock diffraction at time $t + \Delta t$. The difference between the positions of this point at the beginning and end of the time step provides the transformation between the two frames of reference.

There are several important issues connected with the changes in topology for the tracked waves as they collide and interact. These include the numerical detection and identification of the tracked wave interactions, and the modification to the tracked wave structures needed in order to simulate the

underlying physics of the interactions. See¹⁰ for a more detailed discussion of these issues.

Figure 2 shows a typical simulation of the Richtmyer-Meshkov instability.

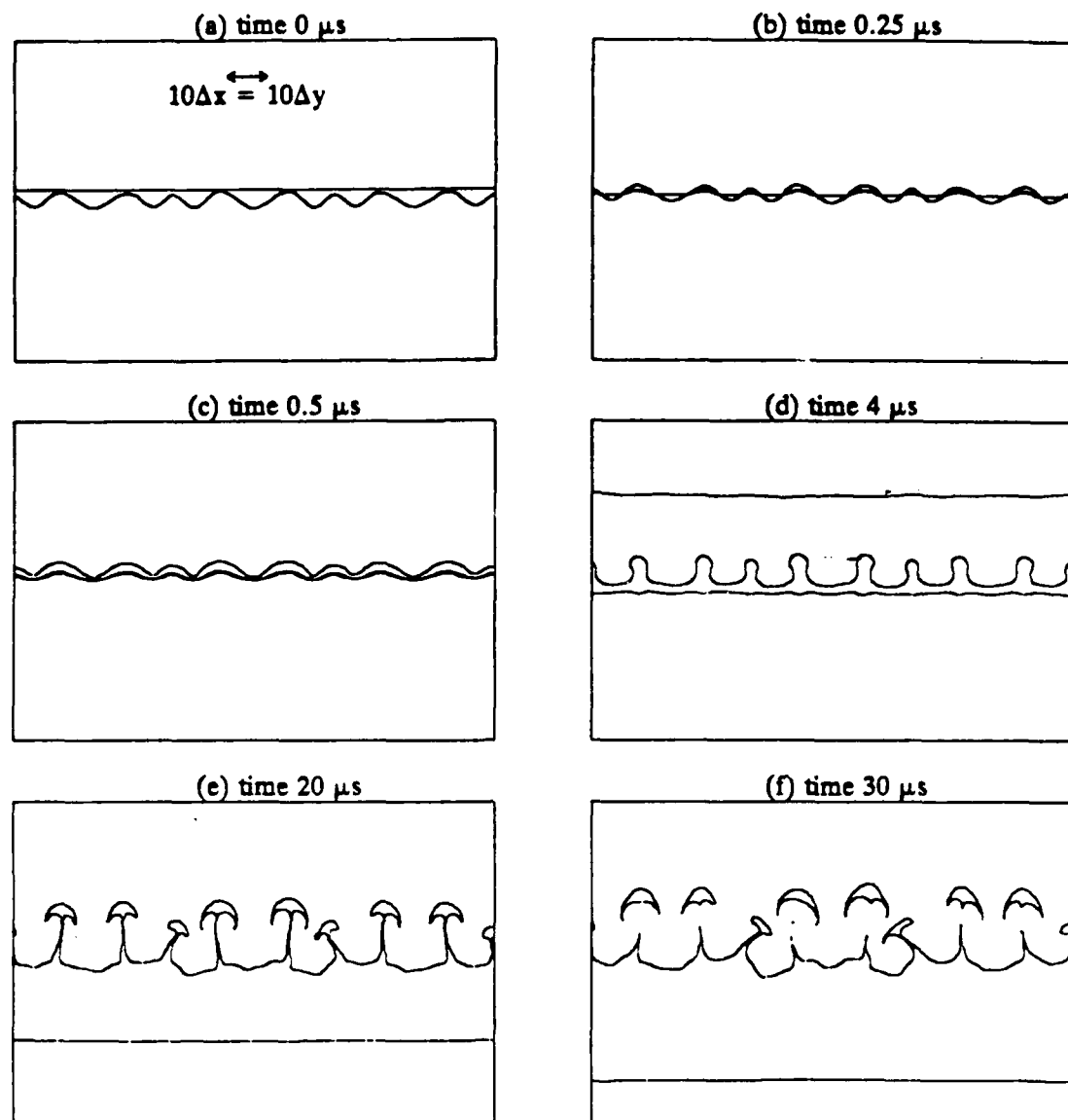


Fig. 2. A series of frames showing a shock in helium ($\gamma = 1.63$) colliding with an air ($\gamma = 1.4$) - helium interface. The pressure in front of the shock is 1 atm. and the pressure behind is 1000 atm.. The density of dry air at 25°C is 0.00118497 g/cc and the density of helium at the same temperature is 0.000101325 g/cc. The grid is 120x80.

4. Results for the Rayleigh-Taylor Instability

We report on preliminary results, to be presented in full in the paper.⁶ The progress concerns step (b): the setting of parameters in the Sharp-Wheeler statistical model and step (c): an analytic and numerical study of this model.

There are two parameters in the two fluid Euler equation (1). One is the Atwood number

$$A = \frac{\rho_b - \rho_a}{\rho_b + \rho_a}$$

or equivalently the density ratio

$$D = \rho_b / \rho_a .$$

The second parameter can be taken as a dimensionless compressibility

$$M = \frac{\sqrt{g\lambda}}{c_b}$$

where λ is a wave length and c_b is the sound speed in the dense fluid. In addition the equations of state (EOS) for the two compressible fluids contain further dimensionless parameters, and are part of the problem definition. Thus problem (b) is to specify

$$c_1 = c_1(A, M, EOS)$$

$$c_2 = c_2(A, M, EOS) .$$

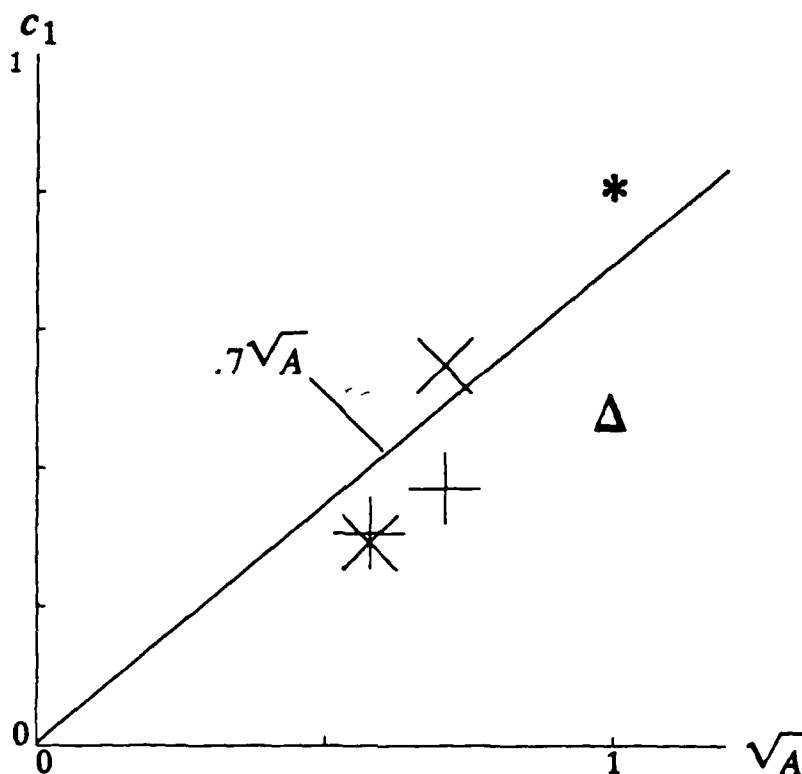


Fig. 3. A plot of the constant c_1 versus the square root of the Atwood ratio for $D = 2$ and 3 ; $M^2 = .5$ (+), 2 (x); and $\gamma = 1.4$. The values of c_1 calculated from the two (*) and three (Δ) dimensional incompressible ($M^2 = 0$, $A = 1$) theories are also shown. The straight line is a curve fit for the data in two dimensions with $c_1 = \alpha \sqrt{A}$. The least squares fit for the free parameter α is $\alpha = .7$.

Computations for a gamma law gas, $\gamma = 1.4$, were performed to determine c_1 . Preliminary results indicate an approximate relationship

$$c_1 \sim \sqrt{A} ,$$

see Figure 3. Careful validation tests for these computations will be reported in reference.⁶ Further computations indicate that the determination of c_2 should be a feasible problem. See Figure 4, where

the merging of two bubbles in a direct simulation of the Rayleigh-Taylor instability are shown. In fact the computation suggests that a more complex process of bubble entrainment is actually occurring.

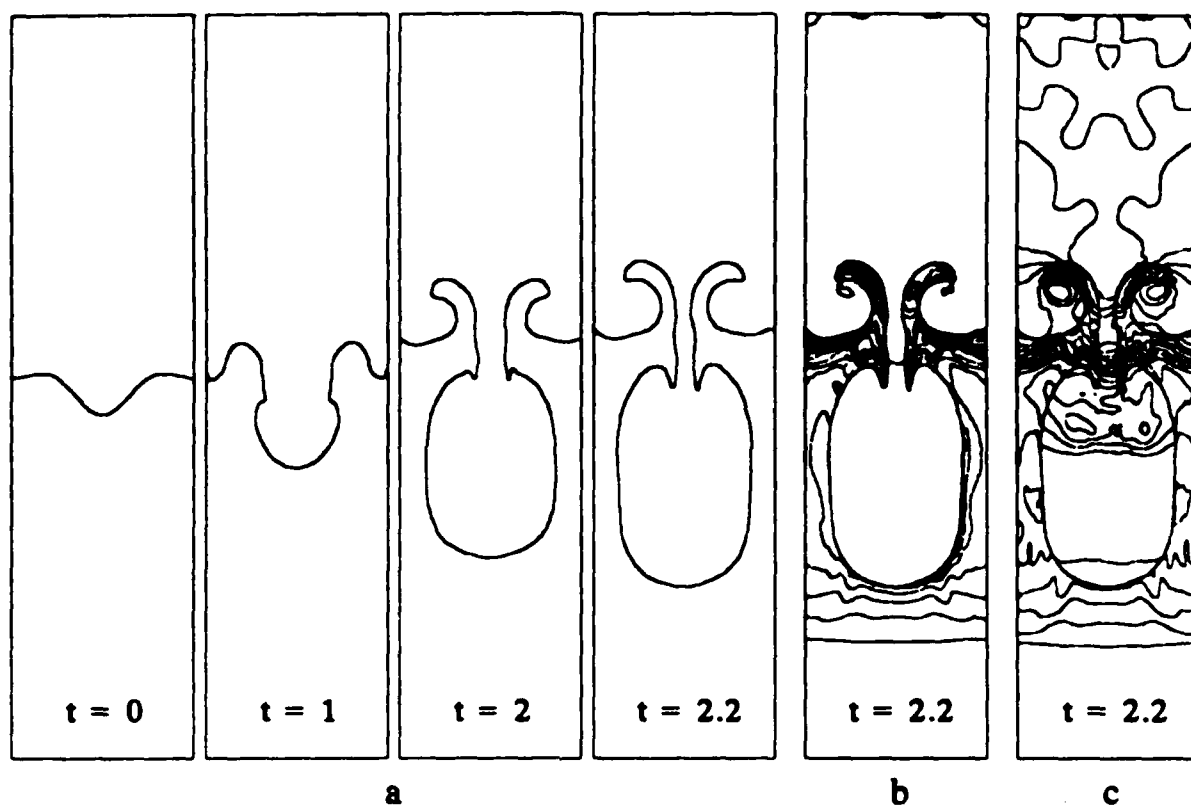


Fig. 4. Plots of the interface position, density and pressure contours of a bubble merger (and entrainment) for $D = 10$, $M^2 = 1.8$, $\gamma = 1.4$ in a computation domain that is 1×4 with 50 by 150 grid blocks. (a) The interface position for successive time steps. (b) The density contour plot. (c) The pressure contour plot. The boundary conditions for the left and right boundaries are periodic. Thus the second bubble is split across these boundaries.

The analytic and numerical analysis of the Sharp-Wheeler model reveals additional structure beyond the simple scaling behavior predicted by Youngs.¹⁵ Because of the merger of bubbles and the transfer of disorder to large scale structures, the bubble interface was predicted^{13,11,15} to move with a mean velocity increasing linearly in t ,

$$h(t) = \alpha g A t^2, \quad v(t) = \dot{h}(t).$$

where A is the Atwood ratio. Youngs predicted a universal value for α and experiments¹² calculated this value as 0.06 (two dimensions) or 0.07 (three dimensions). By examining initial data which contain a length scale, we find evidence for non-universal values of α , at least for a considerable time period. Other elements of structure in the solution of this model are the importance of dynamically generated nearest neighbor correlations in the bubble radii and a possible initial period of exponential growth in the bubble merger process. In Figure 5, we show a series of frames which depict a rising and merging bubble interface based on a numerical solution of the Sharp-Wheeler model.

A full solution of problems (b) and (c) for the Rayleigh-Taylor problem allows a first principles prediction of growth of the bubble interface, with no adjustable parameters. The steps (d) and (e), if

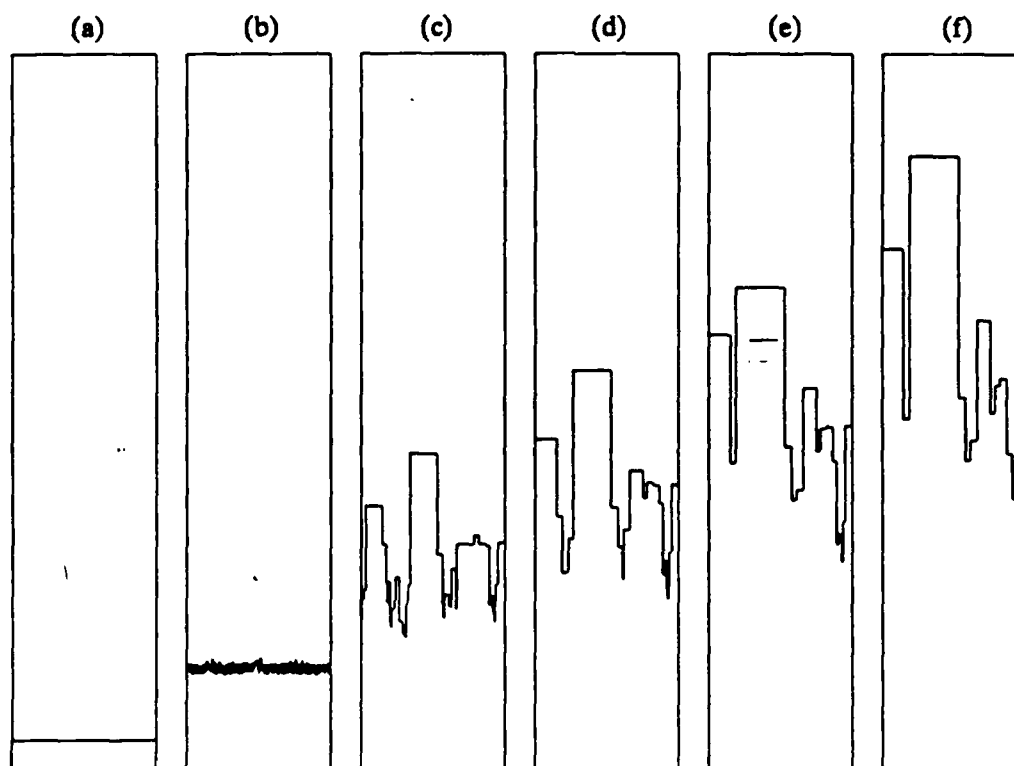


Fig. 5. A sequence of successive sample interfaces generated by the numerical solution of the Sharp-Wheeler bubble growth model.

accomplished, then function as validation of this theory.

Other mechanisms leading to a constant acceleration, $v \sim \alpha t$, of the bubble interface are possible. For an initial time period, the bubbles accelerate (are in free gravitational rise). For the strongly compressible case considered here, the bubbles can attain velocities which are a significant fraction of Mach 1 before reaching terminal velocity. A second possible mechanism for the constant acceleration is that random initial data may contain a mixture of large and small wavelengths. The small wavelengths grow more rapidly at first but then saturate and eventually the initially slower large wavelengths become faster and win out. Thus the large structures may be latent in the initial data, and emerge gradually over time, leading to an acceleration of the bubble interface. Since neither of these mechanisms is present in the Sharp-Wheeler model, their importance would have to be assessed as part of the validation steps (d) and (e).

Finally we comment on three dimensional effects, since the laboratory experiments would almost certainly be three dimensional. The Sharp-Wheeler model as originally formulated applies to three dimensions. The one body interaction constant c_1 can be computed for a radially symmetric bubble. This computation is effectively two dimensional and clearly feasible. The relation of the three dimensional two body interaction constant c_2 to its two dimensional counterpart is less clear, but it is reasonable to assume that these constants are equal to within an order of magnitude.

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